Science
SM358 The Quantum World

SM358

Tutor-Marked Assignment 04

Contents **Cut-off date**

Please send all your answers to the tutor-marked assignment (TMA) to reach your tutor by 12 noon (UK local time) on or before the cut-off date shown on the SM358 website. Your TMAs should be submitted through the eTMA system unless there are difficulties which prevent you from doing so. In these circumstances, you must negotiate with your tutor to get their agreement to submit your assignment on paper. The eTMA system allows for eTMA submission directly to the university 24 hours a day, and either gives you confirmation that your eTMA has been submitted successfully or, if there has been a problem, an error message informing you of the problem and what steps you can take to overcome it. If you submit online you must keep your receipt code in case you need to prove successful submission.

General information about policy and procedure is in the *Assessment Handbook* which you can access from your StudentHome page. However, there are a number of ways in which SM358 eTMA submission differs from what is described there. These are described in the document *Producing eTMAs for Level 3 physics and astronomy modules* on the SM358 website. See also the SM358 *Introduction and Guide* for module-specific information.

Of particular importance is the test submission, TMA 00. This will enable you to familiarize yourself with the system and allow your tutor to check that the format in which you save your TMAs is compatible with their own computer software. It is your responsibility to make sure that you submit documents in a compatible format and we strongly recommend that you submit TMA 00. TMAs submitted in an incorrect format may not be marked.

If you are submitting a paper copy, please allow sufficient time in the post for the assignment to reach its destination on or before the cut-off date. We strongly advise you to use first-class post and to ask for proof of postage. Do not use recorded delivery or registered post as your tutor may not be in to receive it. Keep a copy of the assignment in case it goes astray in the post. You should also include an appropriately completed assignment form (PT3). You will find instructions on how to fill in the PT3 form in the *Assessment Handbook*. Remember to fill in the correct assignment number (04).

This booklet provides advice about submission of TMA answers as well as the questions for TMA04. Although the marks for your assignments do not count directly towards your SM358 result, they are an essential part of your learning and you are required to engage satisfactorily with them. Please refer to the SM358 *Introduction and Guide*, for additional information about the module assessment.

Assignment cut-off dates

The cut-off dates for the assignments provide an important element of pacing for your study of SM358 and they are spread fairly uniformly through the year, leading up to the exam. **You should regard these dates as fixed points**. *Any extension to a TMA cut-off date requires prior permission from your tutor, which may not always be given. Extensions may be granted in exceptional circumstances but it will never be possible to have an extension of more than 3 weeks.* Your tutor will, of course, be willing to discuss with you the best strategies for catching up if you have fallen behind, and should be able to help with questions if you are stuck.

Plagiarism

You are encouraged to discuss the module materials and assignment questions with other students, but the answers to the assignment questions must be your own work. This does not preclude you from making judicious use of material from other sources, but you must acknowledge such use by giving the author's name, the year of publication, the name of the publication in which it appears (or the website address), and the edition or volume number and the page number. However, there is no need to give references for standard equations in the SM358 texts. You are advised to read the University's guidelines on plagiarism, contained in the *Assessment Handbook*, available online from your StudentHome page.

To check that all students are working in a fair and academically appropriate manner, the Open University is currently using some text-comparison software to detect potential cases of plagiarism in work that is submitted for assessment. Details of how this is implemented in this module are given on the SM358 website.

Further general advice on answering SM358 assignment questions is given in the first assignment booklet.

This assignment is related to Chapters 1–5 of Book 3. Your answers for this assignment will provide evidence of your achievement of many of the learning outcomes, as listed in the *Introduction and Guide*, Section 6.5. In particular, this assignment tests *Knowledge and understanding* outcomes 1, 2, 3 and 5, *Cognitive skills* outcomes 1–4 and all three of the *Key skills* outcomes.

Question 1

This question carries 43% of the marks for this assignment and relates mainly to Chapter 2 of Book 3, and particularly Achievements 1.3, 2.8 and 2.10.

This question refers to the Coulomb model of a hydrogen atom, with Hamiltonian operator $\widehat{\mathrm{H}}$, in a state described by the energy eigenfunction

$$\psi_{2,1,-1}(r,\theta,\phi) = \left(\frac{1}{64\pi a_0^3}\right)^{1/2} \frac{r}{a_0}\,\mathrm{e}^{-r/2a_0}\,\sin\theta\,\mathrm{e}^{-\mathrm{i}\phi},$$

where r, θ and ϕ are spherical coordinates and a_0 is the Bohr radius. This eigenfunction has principal quantum number $n=2$, orbital angular momentum quantum number $l=1$ and magnetic quantum number $m=-1$.

(a) Use the given quantum numbers to specify the values of E, L^2 and L_z (the total energy, the square of the magnitude of the orbital angular momentum and the z-component of the orbital angular momentum) in the state described by $\psi_{2,1,-1}$. (6 *marks*)

(b) What feature of the operators $\widehat{\mathrm{H}}$, $\widehat{\mathrm{L}}^2$ and $\widehat{\mathrm{L}}_z$ makes it possible for E, L^2 and L_z to have definite non-zero values in the same hydrogen atom state? Discuss whether any state of a hydrogen atom can exist that has definite non-zero values for all of E, L^2 and L_x. (6 *marks*)

(c) Show that the energy eigenfunction $\psi_{2,1,-1}(r,\theta,\phi)$ is correctly normalized. You may use the standard integrals

$$\int_0^\pi \sin^3\theta\,\mathrm{d}\theta = \frac{4}{3} \quad \text{and} \quad \int_0^\infty r^n \mathrm{e}^{-r/\alpha}\,\mathrm{d}r = n!\,\alpha^{n+1},$$

where $n = 0, 1, 2, \ldots$ and α is any positive constant. (8 *marks*)

(d) The normalized radial function corresponding to $\psi_{2,1,-1}$ is listed in Table 2.1 of Book 3. Use this radial function to show that the radial probability density function in the state described by $\psi_{2,1,-1}$ has its maximum value at $r = 4a_0$. (10 *marks*)

(e) Calculate the expectation values of $1/r$ and $1/r^2$ in the state described by $\psi_{2,1,-1}$. Hence calculate the expectation value and uncertainty of the mutual potential energy of the electron and proton for a hydrogen atom in this state. (13 *marks*)

Question 2

This question carries 25% of the marks for this assignment and relates to Chapter 3 of Book 3, particularly to Achievement 3.7.

Although there is no supporting evidence, suppose for the purposes of this question that there is a deviation from Coulomb's law at very small distances, with the mutual Coulomb potential energy between an electron and a proton being given by

$$V_{\text{mod}}(r) = \begin{cases} -\dfrac{e^2}{4\pi\varepsilon_0}\dfrac{b}{r^2} & \text{for } 0 < r \le b \\[2ex] -\dfrac{e^2}{4\pi\varepsilon_0}\dfrac{1}{r} & \text{for } r > b, \end{cases}$$

where e is the magnitude of the electron charge, ε_0 is the permittivity of free space, r is the electron–proton separation and b is a constant length that is small compared to the Bohr radius but large compared to the radius of a proton.

The Coulomb model of a hydrogen atom (with the potential energy function $V(r) = -e^2/4\pi\varepsilon_0 r$ everywhere) is taken as the unperturbed system. Throughout this question, the perturbed system, with $V(r)$ replaced by $V_{\text{mod}}(r)$, will be called the *modified Coulomb model.*

(a) Specify the perturbation for the modified Coulomb model of a hydrogen atom relative to the unperturbed Coulomb model. (4 *marks*)

(b) Use this perturbation to calculate the first-order correction, $E_1^{(1)}$ to the ground-state energy of a hydrogen atom in the modified Coulomb model, given that the ground-state energy eigenfunction for the unperturbed Coulomb model is

$$\psi_{1,0,0}(r,\theta,\phi) = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \mathrm{e}^{-r/a_0},$$

where a_0 is the Bohr radius. You may use the standard integrals

$$\int_0^x \mathrm{e}^{-u}\,\mathrm{d}u = 1 - \mathrm{e}^{-x}$$

$$\int_0^x u\,\mathrm{e}^{-u}\,\mathrm{d}u = 1 - \mathrm{e}^{-x} - x\mathrm{e}^{-x}.$$

(14 *marks*)

(c) Show that your answer to part (b) can be approximated by

$$E_1^{(1)} \simeq -\frac{4b^2}{a_0^2}E_{\text{R}},$$

where $E_{\text{R}} = e^2/8\pi\varepsilon_0 a_0$ is the Rydberg energy. Hence deduce the largest value of b that would be consistent with the fact that the ground-state energy of a hydrogen atom agrees with the predictions of the Coulomb model to one part in a thousand. Express your answer as a numerical multiple of a_0. (7 *marks*)

You may find it useful to note that for $x \ll 1$,

$$\mathrm{e}^{-x} = 1 - x + \frac{x^2}{2} - \dots.$$

Question 3

This question carries 32% of the marks for this assignment and relates to Chapter 5 of Book 3, particularly to Achievements 5.5, 5.8 and 5.9.

(a) Briefly describe the central-field approximation for many-electron atoms (in around 200 words). Your answer should explain why this approximation predicts that atomic orbitals with the same pair of values of n and l, but different values of m, are degenerate.

In the Coulomb model of a hydrogen atom, states with the same value of n but different values of l have the same energy. Explain why many-electron atoms do not exhibit this degeneracy. Give a qualitative argument indicating why atomic orbitals in a many-electron atom have energies that increase as l increases for any fixed value of n. (11 *marks*)

(b) A titanium atom has an excited-state configuration

$$1\mathrm{s}^2\,2\mathrm{s}^2\,2\mathrm{p}^6\,3\mathrm{s}^2\,3\mathrm{p}^6\,4\mathrm{s}^2\,3\mathrm{d}^1\,4\mathrm{p}^1.$$

When residual electron–electron interactions are taken into account, this configuration splits into a number of atomic terms. List these atomic terms, labelled by their L and S quantum numbers, and also give each term an appropriate spectroscopic symbol. Outline your reasoning. (9 *marks*)

(c) Specify the degree of degeneracy of each atomic term in part (b) and confirm that the total number of states associated with all these atomic terms agrees with the number expected from the l and s quantum numbers of the two valence electrons in the given configuration. (8 *marks*)

(d) When the spin–orbit interaction is taken into account in the LS-coupling scheme, the atomic term with $L = 1$ and $S = 1$ splits into a number of atomic levels. Label these atomic levels by their L, S and J quantum numbers, and give each level an appropriate spectroscopic symbol. Outline your reasoning. (4 *marks*)

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